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Processing of the JEFF-3.1.2 Cross Section Library into various formats (ACE, PENDF, GENDF, MATXSR and BOXER) for testing purposes

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Outline

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1. Objectives and planning

By the end of November 2011 : Processing of the JEFF-3.1.2 Cross Section Library with the NJOY code system into various formats for testing purposes, in particular PENDF, GENDF and BOXER

By the end of December 2011: The JEFF-3.1.2 cross section data file is processed into MCNP/ACE application libraries for different temperatures depending on the application needs.

- The nuclides processed are those of the General Purpose Library
- The library at 300K is verified and compared to other available libraries (JEFF-3.1.1, ENDF-B/VII.0 or VII.1) using JANIS and PREPRO codes
- Quality Assurance (QA) procedure used in producing the data library, pointing out any error/mistake found during the analyses.

By the end of January 2012: Processing into JANIS libraries (i.e. PENDF, BOXER formats) of JEFF-3.1.2 and other new evaluated library (e.g. ENDF/B-VII.1, TENDL-2011). The processed data contain gamma production and gas production data, kinematic KERMA factors and total damage energy data.

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1.1 Processing JEFF-3.1.2 in ACE

- NJOY99.364 is used to process JEFF-3.1.2 Cross Section Library
- 11 temperatures files: 300K -… - 1800K

Figure 1. NJOY processing sequence for a formatted neutron library

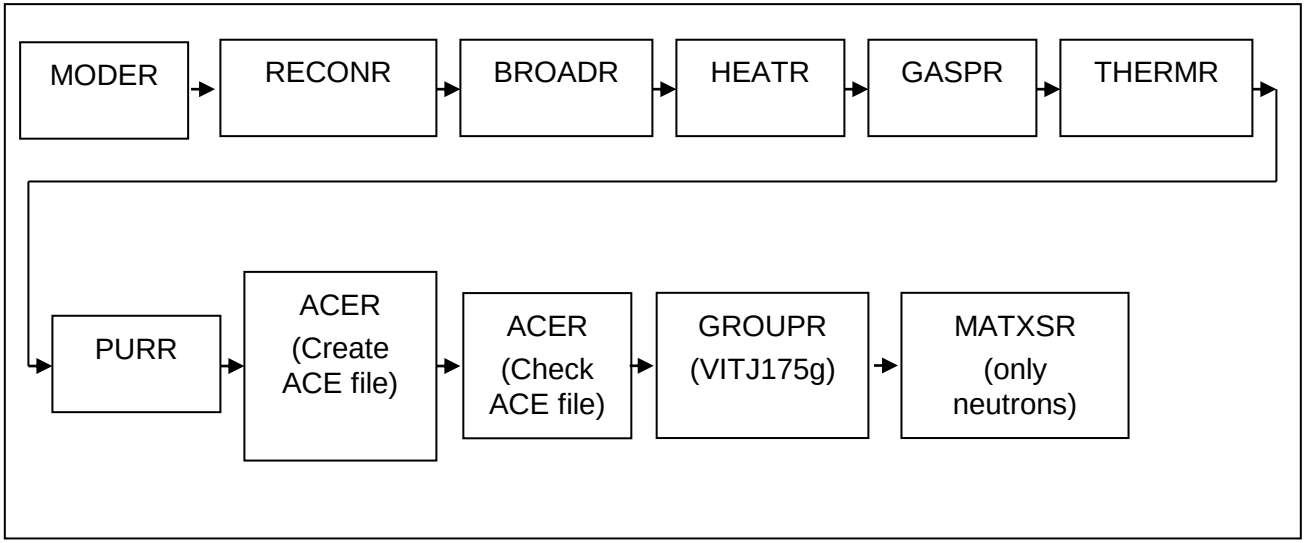

Table 1. Multi-temperature ACE files

#	Temperature (K)	ZAID suffix
1	300	.03c
2	400	.04c
3	500	.05c
4	600	.06c
5	700	.07c
6	800	.08c
7	900	.09c
8	1000	.10c
9	1200	.12c
10	1500	.15c
11	1800	.18c

Example: NJOY input

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-235 from JEFF3.1.2'/
20 9228
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.1.2 PENDF for 92-U-235'/
9228 2/
0.01 0.0 0.01/ err tempr errmax
'JEFF3.1.2: 92-U-235'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9228 1 0 0 0./
0.01 -2.0e+6 0.01/ errthn thnmax errmax
300.
0/
heatr / Add heating kerma and damage energy
21 23 24/
9228 7 0 0 0 2/
302 303 304 318 402 443 444/
gaspr / Add gas production
21 24 25
thermr / Add thermal scattering data
  0 25 61
0 9228 12 1 1 0 1 221 1/
300.
0.001 4.0
purr / if any
21 61 26
9228 1 5 15 32/ matd ntemp nsigz nbin nladr
300.
1.E+10 1.E+04 1.E+03 1.E+02 1.E+01
0/
```

```
acer / Prepare ACE files
21 26 0 27 28
1 0 1 .03/
'92-U-235 from JEFF3.1.2, NJOY99.364, NEA_Dec2011'/
9228 300.
1 1/
/
acer / Check ACE files
0 27 0 29 30
7 1 1 -1/
/
groupr / Prepare multigroup data for neutrons
21 26 0 31
9228 17  0  2 6 1 5 1/
'92-U-235 from JEFF3.1.2(JEFF3.1.2) NJOY 99.364  NEA DEC2011   '/
300.
1.E+10 1.E+04 1.E+03 1.E+02 1.E+01
3/
3  221 'Free Gas'/
3  251 'mubar'/
3  252 'xi'/
3  253 'gamma'/
3  259 '1/v'/
3  452/
3  455/
5  455/
6/
6  221 'Free Gas'/
0/
0/
matxsr / Produce MATXS file
31 0 41/
1 'JEFF-3.1.2:U235  '/
1 2 2 1
'JEFF3.1.2: 92-U-235 from JEFF3.1.2'/
'Processed by NJOY-99.364 at NEA DEC2011 '/
'n' /
175
'nscat' 'ntherm' /
1 1/
1 1/
u235   9228/
stop
```

ACE files

Table 2. Extract of JEFF-3.1.2 ACE library at 300K

#	Nuclide	ZAID	PT Tables JEFF3.1.1	PT Tables JEFF3.1.2	ACE filename	XSDIR filename
1	1-H - 1	1001.03c	-		H1.ACE	H1.DIR
...	...	...	...	…	...	...
334	92-U -235	92235.03c	ptable	(c)	U235.ACE	U235.DIR
...	...	...	...	…	...	...
337	92-U -238	92238.03c	ptable	ptable	U238.ACE	U238.DIR
...	...	...	...	…	...	...
340	93-Np-237	93237.03c	-(a)		Np237.ACE	Np237.DIR
341	93-Np-238	93238.03c	-(a)	(c)	Np238.ACE	Np238.DIR
...	...	...	...	…	...	...
345	94-Pu-238	94238.03c	ptable	(d)	Pu238.ACE	Pu238.DIR
346	94-Pu-239	94239.03c	ptable	ptable	Pu239.ACE	Pu239.DIR
347	94-Pu-240	94240.03c	ptable	(c)	Pu240.ACE	Pu240.DIR
348	94-Pu-241	94241.03c	ptable	ptable	Pu241.ACE	Pu241.DIR
349	94-Pu-242	94242.03c	ptable	ptable	Pu242.ACE	Pu242.DIR
350	94-Pu-243	94243.03c	ptable	(c)	Pu243.ACE	Pu243.DIR
...	...	...	...	…	...	...
353	95-Am-241	95241.03c	ptable	(c)	Am241.ACE	Am241.DIR
...	...	...	...	…	...	...
374	98-Cf-250	98250.03c	ptable	(c)	Cf250.ACE	Cf250.DIR
375	98-Cf-251	98251.03c	ptable	(c)	Cf251.ACE	Cf251.DIR
376	98-Cf-252	98252.03c	-(a)	(c)	Cf252.ACE	Cf252.DIR
377	98-Cf-254	98254.03c	-		Cf254.ACE	Cf254.DIR
378	99-Es-253	99253.03c	-(a)	(c)	Es253.ACE	Es253.DIR
...	...	...	...	…	...	...
381	100-Fm-255	100255.03c	-		Fm255.ACE	Fm255.DIR

(a).Originally, JEFF3.1.1 includes *ptable* option, but it was been eliminated according section 2.3.2.

(c) JEFF3.1.2 includes *ptable* option with some problems according section 2.3.2. This work recommends to use these PTABLES, but it should be revised in future evaluations.

(d) This ptable has been eliminated due to problems in MCNP code.

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Scattering Thermal ACE files

Table 3. Information on the JEFF-3.1.2 Thermal Scattering ACE library at different temperatures

Temp (K)	Hydrogen bound in water	Hydrogen bound in polyethylene	Hydrogen bound in ZrH	Graphite	D bound in D2O	Be
293.6	lw00.32t	pol00.32t	hzr00.32t	gr00.32t	hw00.32t	be00.32t
323	lw01.32t				hw01.32t	
350		pol01.32t				
373	lw02.32t				hw02.32t	
400			hzr01.32t	gr01.32t		be01.32t
423	lw03.32t				hw03.32t	
473	lw04.32t				hw04.32t	
500			hzr02.32t	gr02.32t		be02.32t
523	lw05.32t				hw05.32t	
573	lw06.32t				hw06.32t	
600			hzr03.32t	gr03.32t		be03.32t
623	lw07.32t					
643					hw07.32t	
647	lw08.32t					
700			hzr04.32t	gr04.32t		be04.32t
800	lw09.32t		hzr05.32t	gr05.32t		be05.32t
1000	lw10.32t		hzr06.32t	gr06.32t		be06.32t
1200			hzr07.32t	gr07.32t		be07.32t
1600				gr08.32t		
2000				gr09.32t		
3000				gr10.32t		

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1.2 Processing to JANIS & BOXER

Figure 2. NJOY processing sequence for a JANIS neutron library into BOXER format

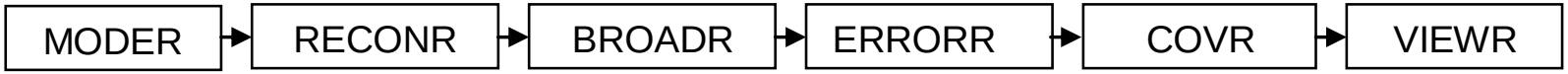
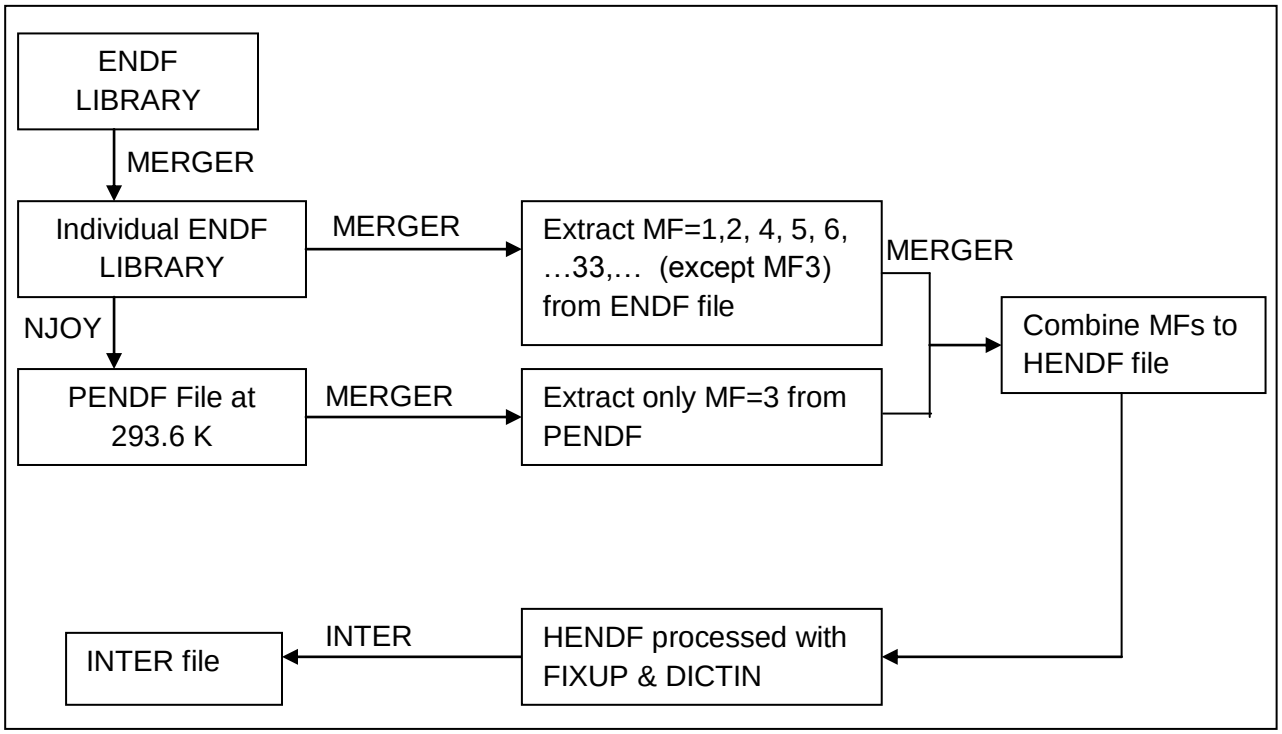


Figure 3. Flowchart of processing JANIS library from ENDF tapes



Example: NJOY

Figure 4. Sample input data of Ac225 (MAT=8925) to generate JANIS library

```
moder /tape20 from MERGER
20 21
reconr /Reconstruct XS data
21 22
' PENDF tape          ' /
8925 2/
.005 0. 0.005/
' MAT=ac225       ENDF Library:          JEFF-3.1.2   ' /
' Processed by NJOY99.364+NEA, NEA Jan12   '/
0/
broadr /Doppler broaden XS
21 22 23
8925 1 0 0 0.
.005 -10.0e+6 0.005/
 293.6
0/
gaspr /Gas production
21 23 24
thermr / Add thermal scattering data
 0 24 25
 0 8925 12 1 1 0 1 221 0
 293.6
0.005 5.0
heatr / Add heating kerma and damage energy
21 25 26/
   8925 2 0 0 0 2/
 443 444/
stop
```

Figure 5. Sample input data of Au197 (MAT=7925) to generate JANIS library in BOXER format

```
moder / Extract/convert neutron evaluated data
1 21
'79-Au-197 from JEFF3.1.2'/
20 7925
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.1.2 PENDF for 79-Au-197'/
7925 2/
                79. 0.0 0.01/ err tempr errmax
,JEFF3.1.2: 79-Au-197'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
7925 1 0 0 0./
0.01 -10.0e+6 0.01/ errthn thnmax errmax
300.
0/
error
21 23 0 77/
7925 17 2 1 1/
1 300.0 / mprint temp
0 33  /Procesa Lib 33 de incertidumbres
covr
77 78/
                79. 1
'NEA JEFF-3.1.2 Dec 2011'/
'Processing BOXER NJOY99.364'/
7925 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
7925 0 0 0 /
viewr
79 80/
stop
```

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Covariances files: MF31, ..., MF40

Table 4. Processing JEFF-3.1.2 in BOXER format

MAT	Nuclide	MF31	MF32	MF33	MF34	MF35	MF40
131	1-H - 3	-	-	OK	-	-	-
425	4-Be- 9	-	-	OK	-	-	-
600	6-C - 0	-	-	OK	-	-	-
925	9-F - 19	-	-	OK	-	-	-
1425	14-Si- 28	-	-	OK	-	-	-
2225	22-Ti- 46	-	-	OK	-	-	-
2228	22-Ti- 47	-	-	OK	-	-	-
2231	22-Ti- 48	-	-	OK	-	-	-
2234	22-Ti- 49	-	-	OK	-	-	-
2237	22-Ti- 50	-	-	OK	-	-	-
2300	23-V - 0	-	-	OK	-	-	-
2425	24-Cr- 50	-	-	OK	-	-	-
2431	24-Cr- 52	-	-	OK	OK	-	-
2434	24-Cr- 53	-	-	OK	-	-	-
2437	24-Cr- 54	-	-	OK	-	-	-
2525	25-Mn- 55	-	OK	OK	-	-	-

MAT	Nuclide	MF31	MF32	MF33	MF34	MF35	MF40
2625	26-Fe- 54	-	-	OK	-	-	-
2631	26-Fe- 56	-	-	OK	OK	-	-
2634	26-Fe- 57	-	-	OK	-	-	-
2637	26-Fe- 58	-	-	OK	-	-	-
2725	27-Co- 59	-	-	OK	-	-	-
2825	28-Ni- 58	-	-	OK	OK	-	-
2831	28-Ni- 60	-	-	OK	OK	-	-
2834	28-Ni- 61	-	-	OK	-	-	-
2837	28-Ni- 62	-	-	OK	-	-	-
2843	28-Ni- 64	-	-	OK	-	-	-
2925	29-Cu- 63	-	-	OK	-	-	-
2931	29-Cu- 65	-	-	OK	-	-	-
3925	39-Y - 89	-	-	OK	-	-	-
4025	40-Zr- 90	-	-	OK	-	-	-
4125	41- Nb-93	-	-	OK	-	-	OK
7525	75-Re-185	-	-	OK	-	-	-
7531	75-Re-187	-	-	OK	-	-	-
7925	79-Au-197	-	-	OK	-	-	-
9222	92-U -233	OK	OK	OK	OK	OK	-
9228	92-U -235	OK	-	-	-	-	-
9543	95-Am-241	-	-	-	-	-	OK

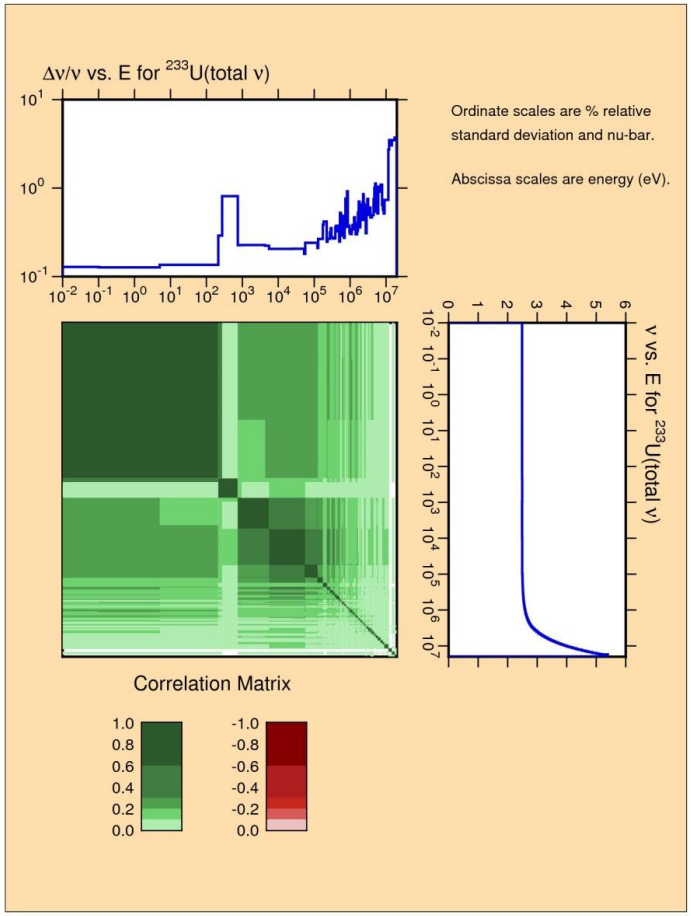
Isotopes with problems to be processed with NJOY99.364:

- Be9, Si28, Fe54, Nb93, U233

Processing U233-MF31

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-233 from JEFF3.1.2'/
20 9222
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.1.2 PENDF for 92-U-233'/
9222 2/
0.01 0.0 0.01/ err tempr errmax
'JEFF3.1.2: 92-U-233'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9222 1 0 0 0./
0.01 -10.0e+6 0.01/ errthn thnmax errmax
300.
0/
groupr / Prepare multigroup data for neutrons
21 23 0 24
9222 17  0  2 6 1 1 1/
'(JEFF3.1.2) NJOY99.364  NEA DEC2011 '/
300.
1.E+10
3/
3  452/
3  455/
3  456/
5  455/
0/
0/
errorr
21 0 24 77/
9222 17 2 1 1/
0 31  /Processing MF31
covr
77 78/
3 1
'NEA JEFF-3.1.2 Dec 2011'/
'Processing BOXER NJOY99.364'/
9222 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9222 0 0 0 /
viewr
79 80/
stop
```

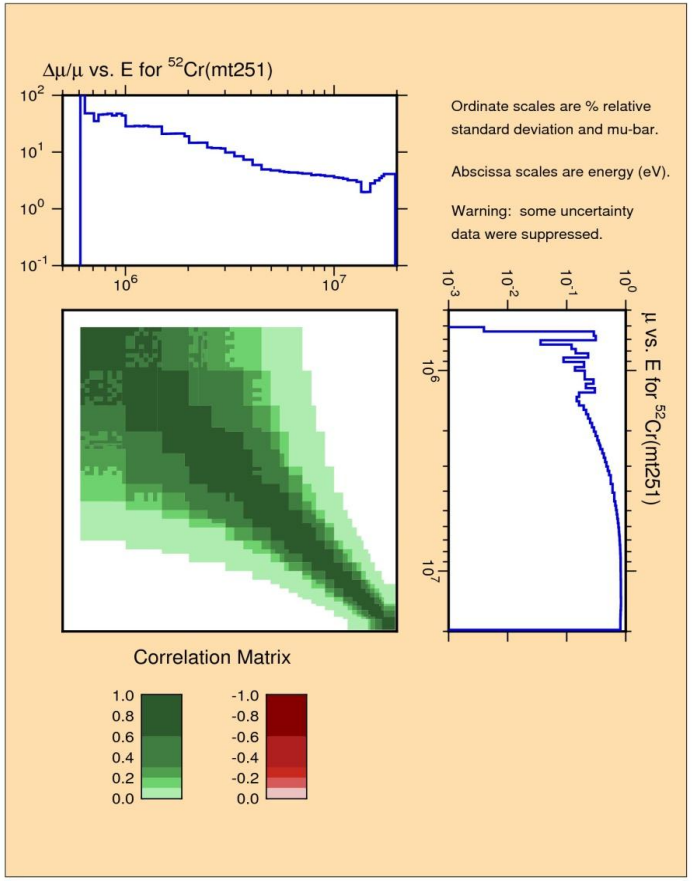
Figure 6. Processing MF31- ^{233}U



Processing Cr52-MF34

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-233 from JEFF3.1.2'/
20 9222
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.1.2 PENDF for 92-U-233'/
9222 2/
0.01 0.0 0.01/ err tempr errmax
'JEFF3.1.2: 92-U-233'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9222 1 0 0 0./
0.01 -10.0e+6 0.01/ errthn thnmax errmax
300.
0/
errorr
21 23 0 77/
9222 17 2 1 1/
1 300.0 / mprint temp
0 34  /Processing MF34
covr
77 78/
3 1
'NEA JEFF-3.1.2 Dec 2011'/
'Processing BOXER NJOY99.364'/
9222 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9222 0 0 0 /
viewr
79 80/
stop
```

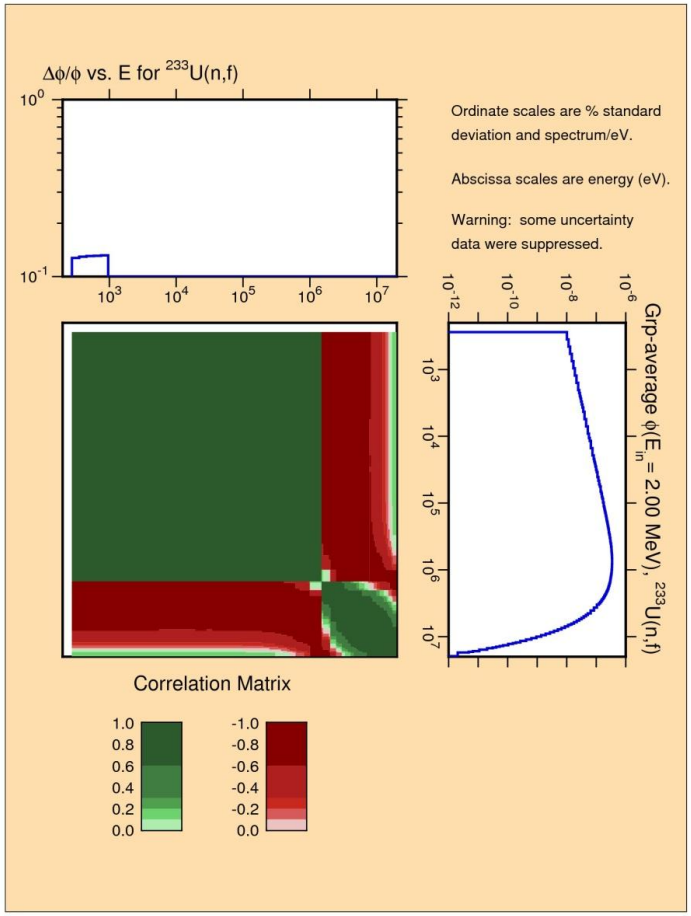
Figure 7. Processing MF34- ^{52}Cr



Processing U233-MF35

```
moder / Extract/convert neutron evaluated data
1 21
'92-U-233 from JEFF3.1.2'/
20 9222
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.1.2 PENDF for 92-U-233'/
9222 2/
0.01 0.0 0.01/ err tempr errmax
'JEFF3.1.2: 92-U-233'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9222 1 0 0 0./
0.01 -10.0e+6 0.01/ errthn thnmax errmax
300.
0/
groupr / Prepare multigroup data for neutrons
21 23 0 24
9222 17  0  2 6 1 1 1/
'(JEFF3.1.2) NJOY99.364  NEA DEC2011 '/
300.
1.E+10
3/
3  452/
3  455/
3  456/
5   18/
0/
0/
errorr
21 0 24 77/
9222 17 2 1 1/
0 35  /Procesing MF35
covr
77 78/
3 1
'NEA JEFF-3.1.2 Dec 2011'/
'Processing BOXER NJOY99.364'/
9222 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9222 0 0 0 /
viewr
79 80/
stop
```

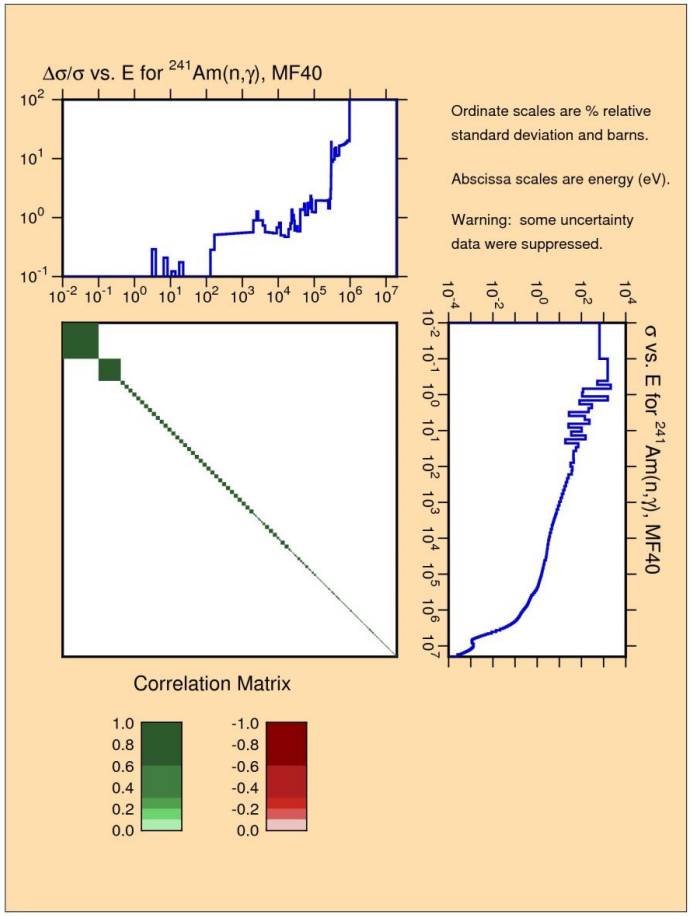
Figure 8. Processing MF35- ^{233}U



Processing Am241-MF40

```
moder / Extract/convert neutron evaluated data
1 21
'95-Am-241 from JEFF3.1.2'/
20 9543
0/
reconr / Reconstruct XS for neutrons
21 22
'JEFF3.1.2 PENDF for 95-Am-241'/
9543 2/
0.01 0.0 0.01/ err tempr errmax
'JEFF3.1.2: 95-Am-241'/
'Processed by NJOY99.364, NEA_Dec2011'/
0/
broadr / Doppler broaden XS
21 22 23
9543 1 0 0 0./
0.01 -10.0e+6 0.01/ errthn thnmax errmax
300.
0/
groupr / Prepare multigroup data for neutrons
21 23 0 24
9543 17  0  2 6 1 1 1/
'(JEFF3.1.2) NJOY99.364  NEA DEC2011 '/
300.
1.E+10
3/
3  452/
3  455/
3  456/
5   18/
0/
0/
errorr
21 0 24 77/
9543 17 2 1 1/
0 40  /Procesa Lib 33 de incertidumbres
covr
77 78/
3 1
'NEA JEFF-3.1.2 Dec 2011'/
'Processing BOXER NJOY99.364'/
9543 0 0 0 /
covr
77 0 79/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9543 0 0 0 /
viewr
79 80/
stop
```

Figure 9. Processing MF40- ^{241}Am



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Problems processing: Be-9

ERRORR module stopped the execution. In JEFF-3.1.2, Be-9 includes covariance data (MF33) for: MT875, ..., MT890 (channels given for alpha emission). However, ERRORR module is not able to process this information:

```
***error in errorr***illegal mt gt 870.
```

See, line in ERRORR.f

```
121 if (mt.gt.870) call error('errorr','illegal mt gt 870.',' ')        errorj.483
```

Problems processing MF32/MF33: Fe-54

An error in **COVR** module stopped the execution.

```
***error in press***matrix not symmetric
   i160 j159 xa(i,j)=  2.2350E-31 xa(j,i)=  0.0E+00
```

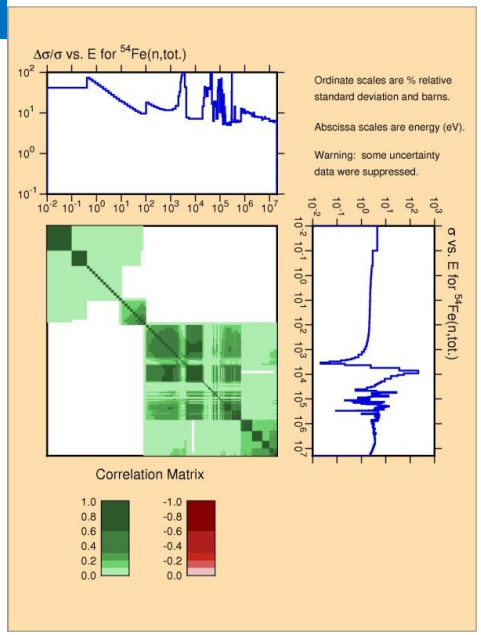

Figure 10. Processing MF33- ^{54}Fe

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Problems processing: Si-28

NJOY has found “nlump=2”, but it fails when looking for “lmt”. The problem in the processing of this material is the definition of MF33 with lumped reaction MT851 and MT852.

```
- MT52 and MT53: Our cross sections for MT 851 were split into     1425 1451   77
  these two components according to the calculated cross           1425 1451   78
  section ratios of ENDF/B-VI.5.                                   1425 1451   79
- MT 54-66: The cross sections for MT 852 were split in the        1425 1451   80
  same way as MT 851.                                              1425 1451   81
```

Where, MF52,...MF66 are already defined. So, lumped MF33/MT851 and MF33/852 are not related with them. According with this sentence, it can be solved deleting and changing these MF33/52-66 sections.

```
 1.402800+4 2.773700+1          0          851          0          0142533 52    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          851          0          0142533 53    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 54    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 55    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 56    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 57    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 58    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 59    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 60    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 61    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 62    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 63    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 64    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 65    1
                                                                    142533  099999
 1.402800+4 2.773700+1          0          852          0          0142533 66    1
                                                                    142533  099999
```

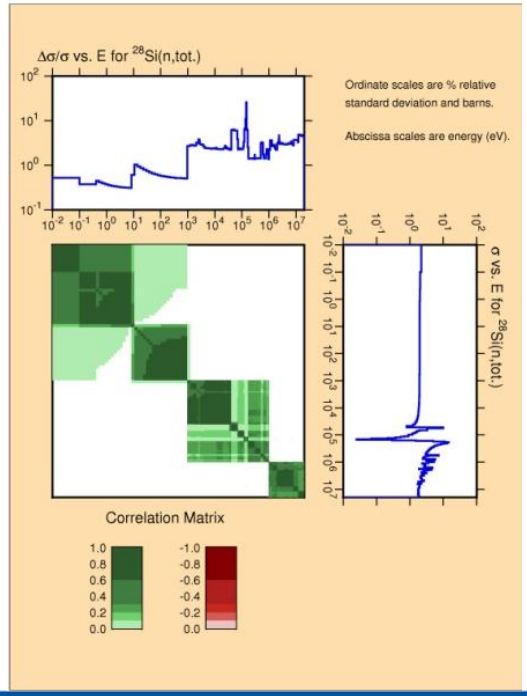

Figure 11. Processing MF33- ^{28}Si

Problems processing: U-233

```
moder
1 71
'moder for selected material'
20  9222
0/
moder
1 21
'moder for selected material'
20  9222
0/
reconr
21 24
'PENDF from New EAF-ENDF TENDL2010'/
 9222 /
0.1 0.0 0.20 1.0e-8 9/
0/
broadr
21 24 25
 9222 1 0 1 0.
0.1 /
300.0
0/
errorr
21 25 0 27 0 71/
9222 17 2 1 1/
1 300.0 / mprint temp
 0 33  /Procesa Lib 33 de incertidumbres
9228 18 9228 102/
0/
covr
27 57/
 3 1
'JEFF-3.1.2'/
'Processing BOXER'/
9222 0 0 0 /
covr
27 0 37/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9222 0 0 0 /
viewr
37 38/
stop
```

NJOY fails due to an error in defining MF32. This problem is solved changing at resonance energies some AJI's now matching with MF2/MT151 (accepted in **JEFF312N9222_0.ASC**)

---message from resprx_rrr_lcomp12---no scattering radius uncertainty

```
7803,7805c7803,7805
< -2.810000+0 2.000000+0 9.795800-4 9.418600-2 3.810800-3 1.357300+0922232151    7
<  1.698200-1 1.000000+0 1.491300-7 6.502000-2 5.587800-2-1.351300-3922232151    8
<  4.401100-1 2.000000+0 1.526300-6 9.144900-4 2.317600-1 1.106800-1922232151    9
---
> -2.810000+0 3.000000+0 9.795800-4 9.418600-2 3.810800-3 1.357300+0922232151    7
>  1.698170-1 3.000000+0 1.491300-7 6.502000-2 5.587800-2-1.351300-3922232151    8
>  4.401140-1 2.000000+0 1.526300-6 9.144900-4 2.317600-1 1.106800-1922232151    9
...
```

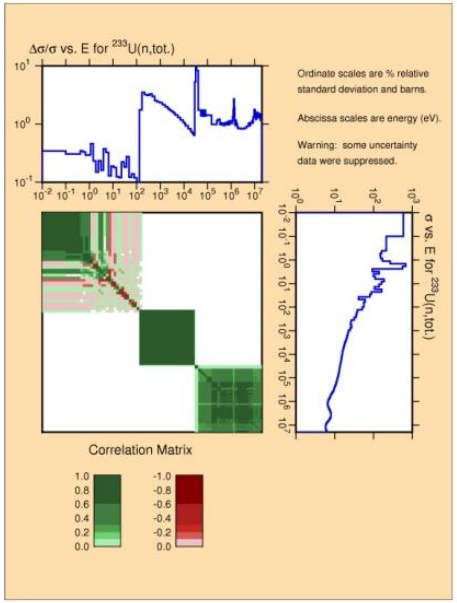

Figure 12. Processing MF33- ^{233}U

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Problems processing: Nb-93

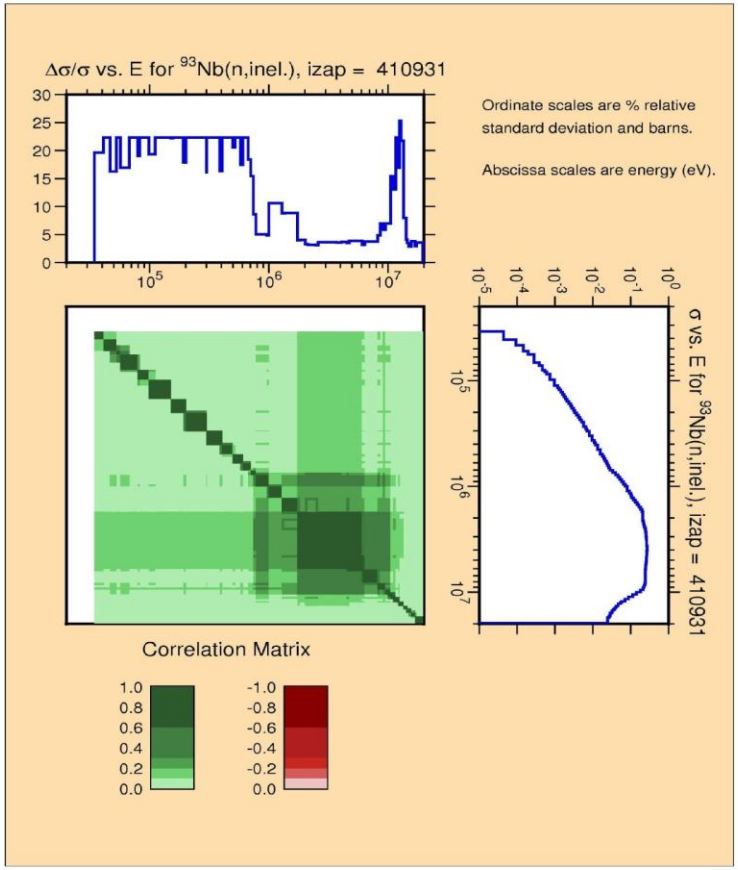
IZAP value fixed in MF10/MT4 and MF40/MT4

```
...
                                                                  4125 0  0     0
 4.109300+4 9.210510+1          0          0          1          0412510  4     1
 0.000000+0-3.082000+4      41093          1          1         32412510  4     2
         32          2                                          412510  4     3
 3.115000+4 0.000000+0 4.000000+4 6.053000-5 5.000000+4 1.513000-4412510  4     4
 6.000000+4 2.522000-4 8.000000+4 5.246000-4 1.000000+5 8.676000-4412510  4     5
....
....
                                                                  4125 0  0     0
 4.109300+4 9.210510+1          0          0          1          0412540  4     1
 0.000000+0-3.082000+4      41093          1          0          1412540  4     2
 1.000000+1 1.000000+0          0          4          0          1412540  4     3
....
```

(Accepted in **JEFF312N4125_0.ASC**)

(*by C. Dean and A. Trkov*)

Figure 13. Processing MF33- ^{93}Nb



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1.3 “Small” changes in NJOY99.364

1) Typo-errors in GASPR

```
*i gaspr.300
      if (mth.ge.154.and.mth.le.159) izg=1
      if (mth.ge.162.and.mth.le.200) izg=1
      if (mth.eq.152) izr=izr-5
      if (mth.eq.153) izr=izr-6
...
...
```

2) Definition of some integer*4 variables in MATXSR

3) Closing tapes in ACER

4) Format errors in COVR

```
*/ covr -- nov2011
*/ - processing JEFF-3.1.2
*d covr.1796
     &     1p,e12.4)') i,im1,xa(im1ind,i),xa(iind,im1)
*d covr.1804
     &  1p,e12.4)') i,im1,xa(im1ind,i),xa(iind,im1)
```

5) Dimension of a vector in GAMINR

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Problems processing GENDF

- In the case of **Pb204,** and for MF17(n,3n) reaction, the second branching reaction has an excitation energy level **(ELFS) of 13**. For this reaction, it is identified with the number: "40822033". And, the branching reaction for the ground level (n,3n) is identified with: "40822020". NJOY fails, because it only can read up to 9 ELFS values.

- Problems processing **Es253** with GROUPR module

```
---message from getunr--- Warning, negative URR cross sections found,
check unresr
```

```
moder
20 -21
reconr
-21 -22
'libreria del material 8225'/
8225 1/
.5 0. /
'libreria del material 8225'/
0/
broadr
-21 -22 -23
8225 1 0 1 0.
.5/
 300
0/
gaspr
-21 -23 -34
unresr
-21 -34 -24
8225 1 1 0
 300
1.e10
0/
groupr
-21 -24 0 27 /card1
8225 17 0 2 0 1 1 0 /card2
'libreria del material 8225'/
 300
1.e10
40822040   4 /
40822061   4 /
40822030  16 /
40822036  16 /
40822020  17 /
40822033  17 /
40801990  24 /
40801997  24 /
0/
0/
stop
```

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Processing TENDL-2011 with NJOY

- Empty files Te-117 and Te-128 in TENDL2011 are not processed
- O-14 can not be processed with NJOY nor PREPRO2010
- NJOY is not able to reconstruct pointwise cross sections in PENDF format with RECONR module for:

  Al26, Ar41, B10, Ba146, Be7, Br86, Co58m, Cs138, Cs142, Es254, Ga79, Hg201, Mn55, Mn56, Ni63, Sb124, Sc45, Sn127, Te124, Tl208 (these files were processed with PREPRO2010)

- In addition, NJOY fails processing BOXER format in:

  ERRORR: Ac223, Am242M, Am244M, Au198M, Be10, Be11, Fr220, Fr223, Os192M, Po210, Po211M, Po212M, Ra221, Ra222, Rn219, U229,U233, U235, U238.

  COVR: Cu60, Cu74, Fe62, Ho155, W178

- A patch is proposed to process cross-correlations in TENDL2011 libraries with NJOY

  The problem in the library was reported to the TENDL2011's team. In MF33, to identify cross-material correlations, the "L1" parameter should be IZAP to identify the nuclide to which the data are correlated. In case of cross-correlation for the same material, "L1" MUST be 0.

```
*ident upm2
*/ errorr -- jan2012
*/ - Processing cross-correlations
*d errorj.913
            if (mt1.eq.mts(i).and.
     .         (mat1.eq.matd.or.mat1.eq.mats(i)) ) then
               go to 220
            endif
*d errorj.1752
               if (mt1.eq.mts(i).and.
     .            (mat1.eq.matd.or.mat1.eq.mats(i)) ) then
                     iyp=i
               endif
```

NJOY patch to process MF33 self cross correlations in TENDL2011

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2. QA procedure

2.1 Comparison & visualization
2.2 Warnings & messages in NJOY and PREPRO
2.3 PREPRO versus NJOY: At low energy, resonances, …
2.4 JEFF-3.1.2 versus ENDF/B-VII.0 - ENDF/B-VII.1
2.5 INTER and BROADR calculation at 293.6K

2.1 QA procedure: comparison & visualization

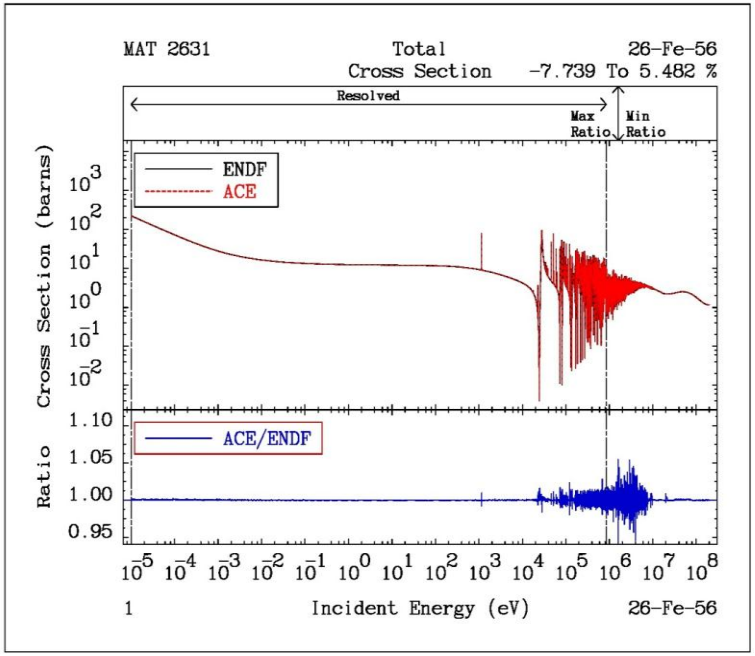

Figure 14. Example of Q&A with ACELST code Fe-56

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2.2 QA: Warnings & Messages

- Checking PREPRO Warnings and messages

- Checking NJOY output messages for each material

- Checking ACE libraries

There are a number of possible problems or abnormalities with the PTs that can be directly noticed for some isotopes **[**W. Haeck,, **ALEPH-DLG]**:

- Probability bins with a probability of 0, these bins will not be sampled so it can be accepted
- Zero cross section values (either for the entire bin or for specific reactions)
- "Negative cross section values"

11-Na-22	18-Ar-36	42-Mo-95	44-Ru-101	46-Pd-105
46-Pd-110	47-Ag-109	58-Ce-141	60-Nd-144	60-Nd-145
60-Nd-148	62-Sm-144	62-Sm-147	62-Sm-152	66-Dy-161
75-Re-185	75-Re-187	92-U-235	93-Np-238	94-Pu-240
94-Pu-243	95-Am-241	98-Cf-250	98-Cf-251	98-Cf-252
99-Es-253				

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2.3 PREPRO vs NJOY: At low energy

Figure 15. Total cross-section Tl-nat

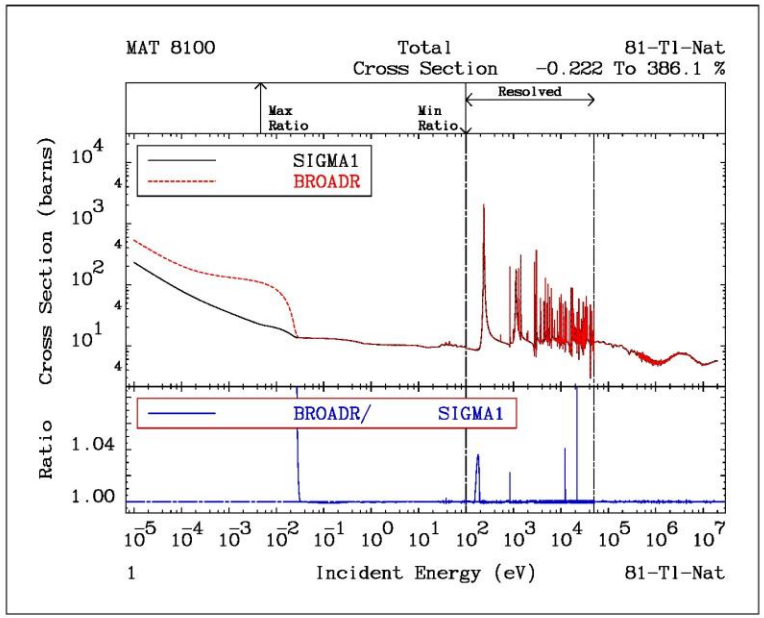
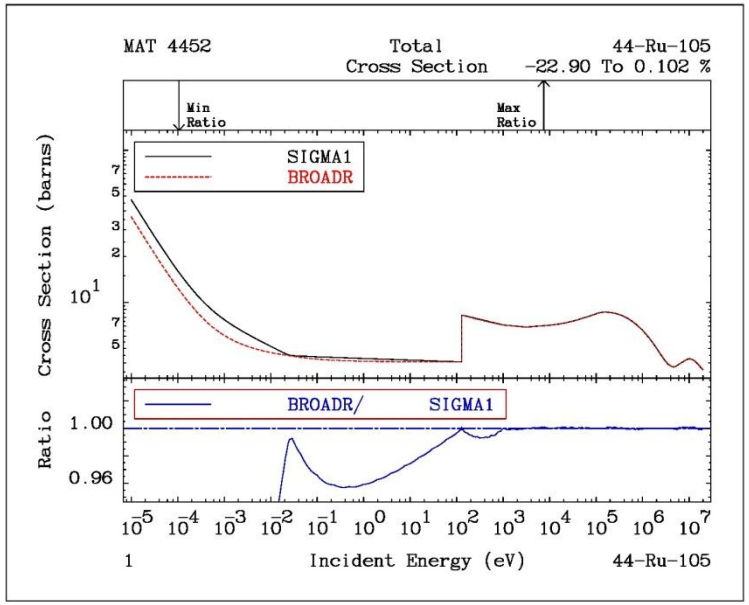


Figure 16. Total cross-section Ru-105



SIGMA1 code uses a log-log interpolation at low energy

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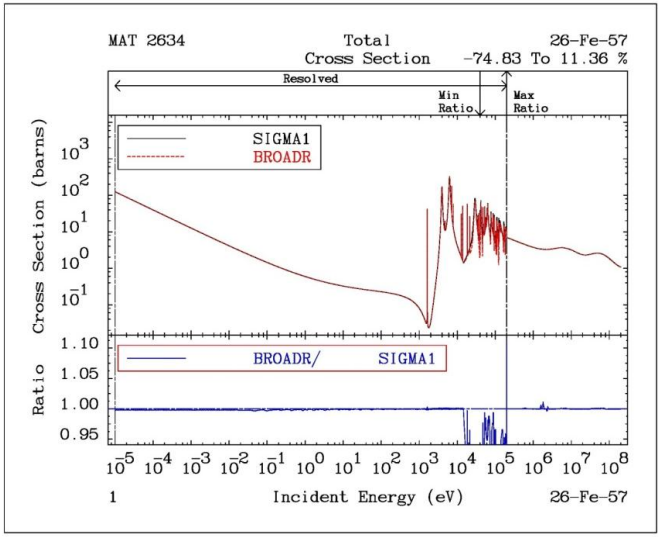
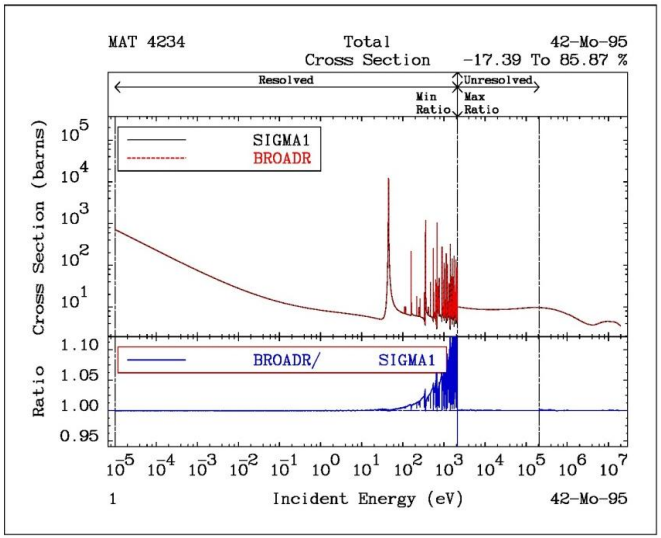
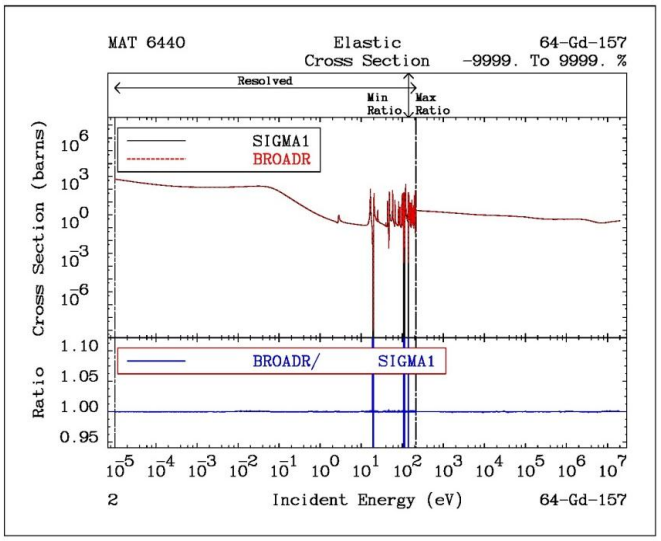
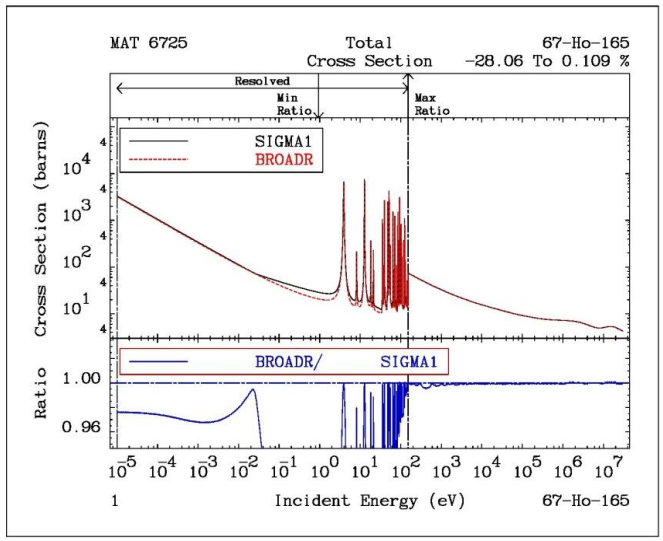
PREPRO vs NJOY: Resonances









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2.4 JEFF-3.1.2 vs ENDF/B-VII.0-VII.1

Figure 17. Total cross-section Hf-176

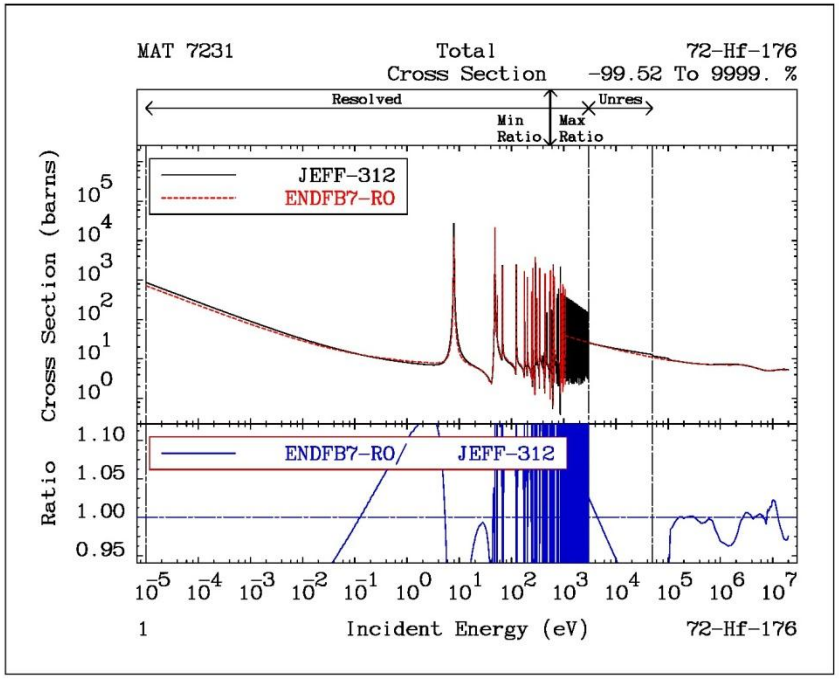
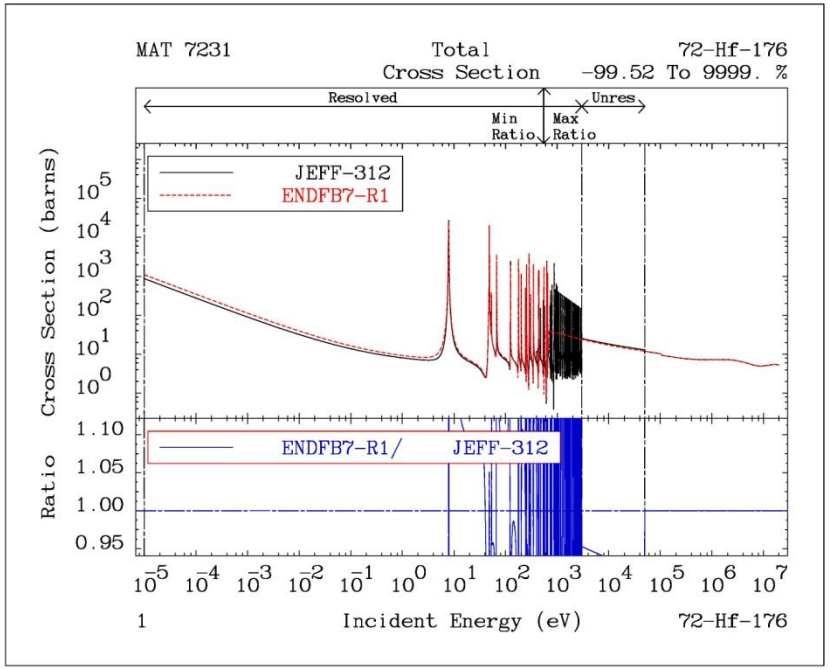


Figure 18. Total cross-section Hf-176



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2.5 INTER calculation at 293.6K

Material number (MAT) = 721760 NAME= hf176

LIBRARY	Z	A	LISO	LFS	MT	Reaction	Sig(2200)	Sig(Ezero)	Avg-Sigma	G-fact	Res Integ	Sig(Fiss)	Sig(E14)
EAF-2007	72	176	0		1	Total	1.40636E+01	1.40536E+01	1.4093E+01	1.00285	6.09825E+02	1.54606E-01	1.96095E+00
ENDFB-6.8	72	176	0		1	Total	2.04851E+01	2.04753E+01	2.1353E+01	1.04316	7.70696E+02	7.02399E+00	5.30000E+00
ENDFB-7.0	72	176	0		1	Total	2.04851E+01	2.04753E+01	2.1353E+01	1.04316	7.70696E+02	7.02399E+00	5.30000E+00
ENDFB-7.1	**72**	**176**	**0**		**1**	**Total**	**2.69430E+01**	**2.69278E+01**	**2.7685E+01**	**1.02832**	**1.11627E+03**	**7.13610E+00**	**5.37211E+00**
JEF-2.2	72	176	0		1	Total	1.85566E+01	1.85466E+01	1.9159E+01	1.03325	9.71128E+02	6.98886E+00	5.67229E+00
JEFF-3.0	72	176	0		1	Total	2.90479E+01	2.90313E+01	2.9811E+01	1.02704	1.42899E+03	7.22047E+00	5.37211E+00
JEFF-3.0A	72	176	0		1	Total	1.40636E+01	1.40537E+01	1.4093E+01	1.00283	6.10193E+02	9.53312E-02	1.96144E+00
JENDL-3.3	72	176	0		1	Total	2.90479E+01	2.90313E+01	2.9811E+01	1.02704	1.42899E+03	7.14147E+00	5.37211E+00
TENDL-2008	72	176	0		1	Total	2.88987E+01	2.88820E+01	2.9623E+01	1.02585	1.12074E+03	7.04831E+00	5.37230E+00
TENDL-2011	**72**	**176**	**0**		**1**	**Total**	**2.88980E+01**	**2.88817E+01**	**2.9621E+01**	**1.02578**	**1.13440E+03**	**7.15742E+00**	**5.30539E+00**
JEFF-3.1.1	72	176	0		1	Total	2.68571E+01	2.68419E+01	2.7596E+01	1.02828	1.12113E+03	7.14147E+00	5.37211E+00
JEFF-3.1.2	**72**	**176**	**0**		**1**	**Total**	**2.21498E+01**	**2.21378E+01**	**2.2845E+01**	**1.03215**	**1.04242E+03**	**7.14086E+00**	**5.37211E+00**

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2.7 BROADR calculation at 293.6K

JEFF-3.1.2 has been processed at 293.6 K (.0253 eV), **BROADR computes**:

- fission cross section at thermal
- fission nu-bar at thermal
- capture cross section at thermal
- thermal Maxwellian fission integral
- thermal Maxwellian capture integral
- fission g-factor (deviation from 1/*v*)
- capture g-factor
- thermal alpha integral
- thermal eta integral
- thermal K1 integral
- fission resonance integral
- capture resonance integral

Material number (MAT) = 721760 NAME= hf176

LIBRARY	the fis xs	the fis nb	the cap xs	the cap int	cap res int	the fis int	the fis g-f	the alp int	…
EAF-2007	0.00000E+00	0.00000E+00	1.40640E+01	1.24990E+01	6.10530E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
ENDFB-6.8	0.00000E+00	0.00000E+00	1.37630E+01	1.22170E+01	4.00720E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
ENDFB-7.0	0.00000E+00	0.00000E+00	1.37630E+01	1.22170E+01	4.00720E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
ENDFB-7.1	**0.00000E+00**	**0.00000E+00**	**2.13840E+01**	**1.89990E+01**	**6.94410E+02**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	…
JEF-2.2	0.00000E+00	0.00000E+00	1.40550E+01	1.24920E+01	6.14270E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
JEFF-3.0	0.00000E+00	0.00000E+00	2.34900E+01	2.08860E+01	8.93150E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
JEFF-3.0A	0.00000E+00	0.00000E+00	1.40640E+01	1.24990E+01	6.10670E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
JENDL-3.3	0.00000E+00	0.00000E+00	2.34900E+01	2.08860E+01	8.93150E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
TENDL-2008	0.00000E+00	0.00000E+00	2.34770E+01	2.08550E+01	7.12520E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
TENDL-2011	**0.00000E+00**	**0.00000E+00**	**2.34760E+01**	**2.08530E+01**	**7.13690E+02**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	…
JEFF-3.1.1	0.00000E+00	0.00000E+00	2.13280E+01	1.89490E+01	6.94460E+02	0.00000E+00	0.00000E+00	0.00000E+00	…
JEFF-3.1.2	**0.00000E+00**	**0.00000E+00**	**1.68500E+01**	**1.49650E+01**	**6.33610E+02**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	…

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3. Criticality Validation Suite

- An expanded Criticality Validation Suite, taken from Integral Benchmark Experiments, ICSBEP for Criticality Safety.
- Presented by *R.D. Mosteller, F.B. Brown and B.C. Kiedrowski* in ICNC2011 to test ENDF/B-VII.1β3 containing **119 cases [LA-UR-11-04170]** for a variety of fuels. A comparison with **[NEA/JEFF-3.1.1]** is also performed in this work:
  - ✓ ^{233}U : 18
  - ✓ Highly enriched uranium (HEU) : 40
  - ✓ Intermediate-enriched uranium (IEU): 17
  - ✓ Low-enriched uranium (LEU) : 8
  - ✓ Plutonium : 36
- For each type of fuel, there are cases with a variety of:
  - ✓ Moderators
  - ✓ Reflectors
  - ✓ Spectra
  - ✓ Geometries
- In addition, 4 cases also included in ICSBEP are used for testing purposes:
  - ✓ Np237
  - ✓ Heavy-Water solutions
  - ✓ Very thermal Pu solution
  - ✓ Unmoderated ZEUS benchmark

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^{233}U Benchmarks

					keff				
						LA-UR-11-04170 & ICNC2011, R.D. Mosteller		This work	
Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	ENDF/B-VII.0[*]	ENDF/B-VII.1β3[*]	JEFF-3.1.2	JEFF-3.1.1[**]
Fast	Metal	Spheres	Unreflected	u233-met-fast-001	1.0000±0.0010	0.9996±0.0003	0.9995±0.0003	1.00423±0.00025	1.00384±0.00025
			HEU	u233-met-fast-002-CASE_1	1.0000±0.0010	0.9986±0.0003	0.9990±0.0003	1.00251±0.00026	-
				u233-met-fast-002-CASE_2	1.0000±0.0011	1.0002±0.0003	1.0006±0.0003	1.00404±0.00026	-
			Normal Uranium	u233-met-fast-003-CASE_1	1.0000±0.0010	0.9990±0.0003	0.9996±0.0003	1.00485±0.00026	-
				u233-met-fast-003-CASE_2	1.0000±0.0010	0.9993±0.0003	1.0001±0.0003	1.00481±0.00029	-
				u233-met-fast-006	1.0000±0.0014	0.9987±0.0003	0.9995±0.0003	1.00541±0.00031	1.00509±0.00029
			Tungsten	u233-met-fast-004-CASE_1	1.0000±0.0007	0.9987±0.0003	1.0049±0.0003	1.00521±0.00029	-
				u233-met-fast-004-CASE_2	1.0000±0.0008	0.9954±0.0003	1.0052±0.0003	1.00413±0.00027	-
			Beryllium	u-233-met-fast-005-CASE_1	1.0000±0.0030	0.9963±0.0003	0.9941±0.0003	1.00043±0.00027	-
				u-233-met-fast-005-CASE_2	1.0000±0.0030	0.9956±0.0003	0.9924±0.0003	1.00032±0.00030	1.00011±0.00030
Intermediate	Solution	Sphere	Beryllium	u233-sol-inter-001-case1	1.0000±0.0083	-	0.9848±0.0005	0.98412±0.00049	0.98459±0.00049
Thermal	UO2+ZrO2	Lattice	Water	u233-comp-therm-001-case3	1.0000±0.0024	-	1.0045±0.0005	0.99739±0.00047	0.99871±0.00045
	Solution	Sphere	Unreflected	u233-sol-therm-001-case1	1.0000±0.0031	-	1.0015±0.0003	0.99892±0.00026	-
				u233-sol-therm-001-case2	1.0000±0.0033	-	1.0011±0.0003	0.99832±0.00026	-
				u233-sol-therm-001-case3	1.0000±0.0033	-	1.0009±0.0009	0.99863±0.00025	-
				u233-sol-therm-001-case4	1.0000±0.0033	-	1.0019±0.0003	0.99873±0.00026	-
				u233-sol-therm-001-case5	1.0000±0.0033	-	0.9996±0.0003	0.99736±0.00027	-
				u233-sol-therm-008	1.0000±0.0029	-	1.0012±0.0002	0.99807±0.00018	0.99807±0.00017

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

INDUSTRIALES
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HEU Benchmarks

					keff				
						LA-UR-11-04170 &ICNC2011, R.D. Mosteller		This work	
Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	ENDF/B-VII.0[*]	ENDF/B-VII.1β3[*]	JEFF-3.1.2	JEFF-3.1.1 [**]
Fast	Metal	Spheres	Unreflected	heu-met-fast-001	1.0000±0.0010	0.9997±0.0003	0.9994±0.0003	0.99597±0.00025	0.99696±0.00027
				heu-met-fast-008	0.9989±0.0016	-	0.9957±0.0003	0.99197±0.00026	-
				heu-met-fast-018-case2	1.0000±0.0014	0.9996±0.0003	0.9999±0.0003	0.99643±0.00026	-
			Normal Uranium	heu-met-fast-003-case1	1.0000±0.0050	0.9947±0.0003	0.9948±0.0003	0.99365±0.00030	-
				heu-met-fast-003-case2	1.0000±0.0050	0.9947±0.0003	0.9945±0.0003	0.99349±0.00029	-
				heu-met-fast-003-case3	1.0000±0.0050	0.9995±0.0003	0.9991±0.0003	0.99796±0.00029	-
				heu-met-fast-003-case4	1.0000±0.0030	0.9974±0.0003	0.9971±0.0003	0.99539±0.00029	-
				heu-met-fast-003-case5	1.0000±0.0030	1.0012±0.0003	1.0008±0.0003	0.99980±0.00029	-
				heu-met-fast-003-case6	1.0000±0.0030	1.0019±0.0003	1.0020±0.0003	1.00030±0.00027	-
				heu-met-fast-003-case7	1.0000±0.0030	1.0018±0.0003	1.0018±0.0003	1.00119±0.00028	-
				heu-met-fast-028	1.0000±0.0030	-	1.0032±0.0003	1.00164±0.00030	1.00157±0.00028
			Depleted Uranium	heu-met-fast-014	0.9989±0.0017	0.9976±0.0003	0.9978±0.0003	0.99584±0.00028	-
			Tungsten carbide	heu-met-fast-003-case8	1.0000±0.0050	1.0014±0.0003	1.0082±0.0003	1.00043±0.00030	-
				heu-met-fast-003-case9	1.0000±0.0050	1.0014±0.0003	1.0095±0.0003	1.00231±0.00029	-
				heu-met-fast-003-case10	1.0000±0.0050	1.0050±0.0003	1.0129±0.0003	1.00862±0.00028	-
				heu-met-fast-003-case11	1.0000±0.0050	1.0099±0.0003	1.0166±0.0003	1.01404±0.00029	-
			Nickel	heu-met-fast-003-case12	1.0000±0.0030	-	1.0083±0.0003	1.00229±0.00029	-
			Steel	heu-met-fast-013	0.9990±0.0015	-	0.9975±0.0003	0.99203±0.00026	-
				heu-met-fast-021-case2	1.0000±0.0024	-	0.9969±0.0003	0.99335±0.00029	-
			Duralumin	heu-met-fast-022-case2	1.0000±0.0019	-	0.9977±0.0003	0.99365±0.00028	-
			Aluminium	heu-met-fast-012	0.9992±0.0018	-	0.9982±0.0003	0.99436±0.00029	-
			Graphite	heu-met-fast-019-case2	1.0000±0.0028	-	1.0074±0.0003	1.00335±0.00027	-
			Beryllium	heu-met-fast-009-case1	0.9992±0.0015	0.9976±0.0003	0.9949±0.0003	0.99337±0.00030	-
			Beryllium Oxide	heu-met-fast-009-case2	0.9992±0.0015	0.9967±0.0003	0.9955±0.0003	0.99239±0.00028	-
			Polyethylene	heu-met-fast-011	0.9989±0.0015	-	0.9989±0.0003	0.99533±0.00035	-
				heu-met-fast-020-case2	1.0000±0.0028	-	1.0008±0.0003	0.99751±0.00030	-
			Water	heu-met-fast-004-case1	1.0020±0.0010	-	1.0028±0.0003	0.99556±0.00034	0.99502±0.00034
		Cylinder	Unreflected	heu-met-fast-015	0.9996±0.0017	-	0.9943±0.0003	0.99081±0.00027	-
		Lattice	Paraffin	heu-met-fast-026-case9	1.0000±0.0038	-	1.0037±0.0003	0.98715±0.00031	-

HEU Benchmarks

					keff				
						LA-UR-11-04170 &ICNC2011, R.D. Mosteller		This work	
Spectrum	**Form**	**Shape**	**Moderator and/or Reflector**	**ICSBEP Benchmark name**	**Benchmark**	**ENDF/B-VII.0[*]**	**ENDF/B-VII.1β3[*]**	**JEFF-3.1.2**	**JEFF-3.1.1 [**]**
Intermediate	**UH3**	**Cylinder**	**Natural U**	heu-comp-inter-003-case7	1.0000±0.0047	-	**0.9951±0.0003**	0.99602±0.00036	-
	Metal	**Cylinder**	**Graphite, copper**	heu-met-inter-006-case1	0.9977±0.0008	-	**0.9930±0.0004**	**0.99271±0.00034**	-
				heu-met-inter-006-case2	0.9997±0.0008	-	**0.9960±0.0004**	**0.99439±0.00033**	**0.99440±0.00033**
				heu-met-inter-006-case3	1.0015±0.0009	-	**1.0006±0.0004**	**0.99798±0.00034**	-
				heu-met-inter-006-case4	1.0016±0.0008	-	**1.0075±0.0003**	**1.00584±0.00035**	-
Thermal	**UO2+ZrO2**	**Lattice**	**Water, ThO2**	u233-comp-therm-001-case6	1.0015±0.0028	-	0.9991±0.0004	**0.99831±0.00040**	**0.99751±0.00051**
	Solution	**Sphere**	**Unreflected**	heu-sol-therm-013-case1	1.0012±0.0026	-	**0.9985±0.0003**	0.99956±0.00025	-
				heu-sol-therm-013-case2	1.0007±0.0036	-	0.9975±0.0003	0.99797±0.00028	-
				heu-sol-therm-013-case3	1.0009±0.0036	-	**0.9942±0.0003**	**0.99491±0.00029**	-
				heu-sol-therm-013-case4	1.0003±0.0036	-	**0.9957±0.0003**	**0.99571±0.00030**	-
				heu-sol-therm-032	1.0015±0.0026	-	0.9991±0.0002	0.99954±0.00017	0.99928±0.00017

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

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IEU Benchmarks

					keff				
						LA-UR-11-04170 &ICNC2011, R.D. Mosteller		This work	
Spectrum	**Form**	**Shape**	**Moderator and/or Reflector**	**ICSBEP Benchmark name**	**Benchmark**	**ENDF/B-VII.0[*]**	**ENDF/B-VII.1β3[*]**	**JEFF-3.1.2**	**JEFF-3.1.1[**]**
Fast	**Metal**	**Spheres**	**Unreflected**	ieu-met-fast-003-case2	1.0000±0.0017	-	**1.0029±0.0003**	0.99899±0.00027	0.99879±0.00026
			Steel	ieu-met-fast-005-case2	1.0000±0.0021	-	1.0018±0.0003	**0.99723±0.00027**	-
			Duralumin	ieu-met-fast-006-case2	1.0000±0.0023	-	**0.9957±0.0003**	**0.99232±0.00027**	-
			Graphite	ieu-met-fast-004-case2	1.0000±0.0030	-	**1.0075±0.0003**	**1.00335±0.00028**	**1.00339±0.00027**
		Cylinder	**Unreflected**	ieu-met-fast-001-case1	0.9989±0.0010	-	**1.0009±0.0003**	**0.99786±0.00028**	-
				ieu-met-fast-001-case2	0.9997±0.0010	-	**1.0013±0.0003**	**0.99800±0.00027**	-
				ieu-met-fast-001-case3	0.9993±0.0005	-	**1.0014±0.0003**	**0.99775±0.00029**	-
				ieu-met-fast-001-case4	1.0002±0.0005	-	**1.0015±0.0003**	**0.99774±0.00026**	-
			Normal U	ieu-met-fast-002	1.0000±0.0030	-	0.9991±0.0003	**0.99178±0.00026**	-
			Depleted U	ieu-met-fast-007-case1	1.0049±0.0008	-	1.0049±0.0002	**0.99764±0.00024**	**0.99792±0.00024**
Intermediate	**Plate**	**Lattice**	**Normal U, steel**	mix-met-fast-008-case7	1.0030±0.0025	-	**1.0193±0.0002**	**1.01637±0.00019**	**1.01574±0.00022**
Thermal	**UO2**	**Lattice**	**Water**	ieu-comp-therm-002-CASE_3	1.0017±0.0044	-	1.0045±0.0004	1.00064±0.00031	1.00105±0.00034
	Solution	**Cylinder**	**Unreflected**	leu-sol-therm-007-CASE14	0.9961±0.0009	-	**0.9950±0.0003**	0.99559±0.00033	-
				leu-sol-therm-007-CASE30	0.9973±0.0009	-	0.9977±0.0003	0.99738±0.00030	-
				leu-sol-therm-007-CASE32	0.9985±0.0010	-	**0.9958±0.0003**	**0.99610±0.00029**	-
				leu-sol-therm-007-CASE36	0.9988±0.0011	-	0.9986±0.0003	0.99858±0.00027	0.99877±0.00020
				leu-sol-therm-007-CASE49	0.9983±0.0011	-	0.9975±0.0003	0.99822±0.00028	-

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

INDUSTRIALES
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LEU Benchmarks

					keff				
						LA-UR-11-04170 &ICNC2011, R.D. Mosteller		This work	
Spectrum	**Form**	**Shape**	**Moderator and/or Reflector**	**ICSBEP Benchmark name**	**Benchmark**	**ENDF/B-VII.0[*]**	**ENDF/B-VII.1β3[*]**	**JEFF-3.1.2**	**JEFF-3.1.1[**]**
Thermal	**UO2**	**Lattice**	**UO2 rods, Water**	leu-comp-ther-008-CASE_1	1.0007±0.0016	-	1.0012±0.0003	1.00105±0.00029	-
				leu-comp-therm-008-CASE_2	1.0007±0.0016	-	1.0013±0.0003	1.00119±0.00031	1.00050±0.00030
				leu-comp-therm-008-CASE_5	1.0007±0.0016	-	1.0007±0.0003	1.00046±0.00031	-
				leu-comp-therm-008-CASE_7	1.0007±0.0016	-	1.0003±0.0003	1.00110±0.00030	-
				leu-comp-therm-008-CASE_8	1.0007±0.0016	-	1.0007±0.0003	0.99988±0.00029	-
				leu-comp-therm-008-CASE_11	1.0007±0.0016	-	1.0020±0.0003	1.00117±0.00029	-
	Solution	**Sphere**	**Water**	leu-sol-therm-002-case1	1.0038±0.0040	-	**1.0000±0.0003**	1.00070±0.00026	-
			Unreflected	leu-sol-therm-002-case2	1.0024±0.0037	-	**0.9959±0.0003**	**0.99629±0.00028**	**0.99655±0.00029**

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

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Plutonium Benchmarks

					Keff				
						LA-UR-11-04170 &ICNC2011, R.D. Mosteller		This work	
Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	ENDF/B-VII. 0[*]	ENDF/B-VII. 1β3[*]	JEFF-3.1.2	JEFF-3.1.1[**]
Fast	Metal	Spheres	Unreflected	pu-met-fast-001-CASE_1	1.0000±0.0020	1.0000±0.0003	1.0000±0.0003	0.99951±0.00027	1.00004±0.00025
				pu-met-fast-002-CASE_1	1.0000±0.0020	0.9998±0.0003	0.9999±0.0003	**1.00413±0.00026**	**1.00394±0.00026**
				pu-met-fast-022	1.0000±0.0021	-	0.9983±0.0003	**0.99770±0.00024**	-
			HEU	mix-met-fast-001-CASE_1	1.0000±0.0016	-	0.9993±0.0003	**0.99809±0.00027**	-
				mix-met-fast-003	0.9993±0.0016	-	1.0008±0.0003	0.99971±0.00026	-
			Normal Uranium	pu-met-fast-006	1.0000±0.0030	1.0002±0.0003	0.9995±0.0003	**1.00306±0.00032**	1.00244±0.00031
				pu-met-fast-010-CASE_1	1.0000±0.0018	0.9998±0.0003	1.0001±0.0018	1.00124±0.00029	-
			Depleted Uranium	pu-met-fast-020	0.9993±0.0017	0.9981±0.0003	0.9981±0.0003	1.00069±0.00029	-
			Thorium	pu-met-fast-008-case2	1.0000±0.0006	**0.9978±0.0003**	**0.9977±0.0003**	**1.00316±0.00028**	**1.00242±0.00027**
			Tungsten	pu-met-fast-005-CASE_1	1.0000±0.0013	1.0011±0.0003	**1.0093±0.0003**	**1.00391±0.00030**	-
			Steel	pu-met-fast-025	1.0000±0.0020	-	0.9988±0.0003	**0.99664±0.00027**	-
				pu-met-fast-026	1.0000±0.0024	-	0.9985±0.0003	0.99806±0.00028	-
			Aluminium	pu-met-fast-009-CASE_1	1.0000±0.0027	-	**1.0053±0.0003**	0.99890±0.00028	-
			Graphite	pu-met-fast-023	1.0000±0.0020	-	0.9993±0.0003	0.99853±0.00028	-
			Beryllium	pu-met-fast-018-CASE_1	1.0000±0.0030	0.9993±0.0003	**0.9964±0.0003**	0.99723±0.00029	-
				pu-met-fast-019	0.9992±0.0015	**1.0009±0.0003**	**0.9976±0.0003**	0.99925±0.00029	-
			Polyethylene	pu-met-fast-024	1.0000±0.0020	-	**1.0019±0.0003**	0.99972±0.00029	-
			Water	pu-met-fast-011-CASE_1	1.0000±0.0010	-	1.0002±0.0003	**0.99689±0.00034**	**0.99623±0.00035**
		Cylinder	Beryllium	pu-met-fast-021-case1	1.0000±0.0026	-	1.0021±0.0003	**1.00321±0.00031**	-
			Beryllium Oxide	pu-met-fast-021-case2	1.0000±0.0026	-	**0.9932±0.0003**	**0.99221±0.00030**	-
		Lattice	Unreflected	pu-met-fast-003-case103	1.0000±0.0030	-	0.9981±0.0003	0.99720±0.00030	**0.99711±0.00031**

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Plutonium Benchmarks

					Keff				
						LA-UR-11-04170 &ICNC2011, R.D. Mosteller		This work	
Spectrum	Form	Shape	Moderator and/or Reflector	ICSBEP Benchmark name	Benchmark	ENDF/B-VII.0 [*]	ENDF/B-VII. 1b3[*]	JEFF-3.1.2	JEFF-3.1.1[**]
Intermediate	Mixture	Homog	Hydrogen, graphite	pu-comp-inter-001	1.0000±0.0110	-	1.0116±0.0002	1.00758±0.00026	1.00807±0.00051
Thermal	MOX	Lattice	Water	mix-comp-therm-002-case-pnl30	1.0024±0.0060	-	1.0010±0.0003	0.99898±0.00034	-
				mix-comp-therm-002-case-pnl31	1.0009±0.0047	-	1.0028±0.0003	1.00199±0.00035	-
				mix-comp-therm-002-case-pnl32	1.0042±0.0031	-	1.0032±0.0003	1.00050±0.00034	-
				mix-comp-therm-002-case-pnl33	1.0024±0.0021	-	1.0079±0.0003	1.00615±0.00033	-
				mix-comp-therm-002-case-pnl34	1.0038±0.0025	-	1.0046±0.0003	1.00233±0.00033	-
				mix-comp-therm-002-case-pnl35	1.0029±0.0027	-	1.0068±0.0003	1.00463±0.00031	-
	Solution	Sphere	Unreflected	pu-sol-therm-009-case3a	1.0000±0.0033	-	1.0190±0.0002	1.01415±0.00017	-
				pu-sol-therm-011-CASE_5.16	1.0000±0.0052	-	1.0060±0.0004	1.00404±0.00042	-
				pu-sol-therm-011-CASE_1.18	1.0000±0.0052	-	0.9944±0.0004	0.99130±0.00034	-
				pu-sol-therm-011-CASE_6.18	1.0000±0.0052	-	0.9996±0.0004	0.99737±0.00037	-
				pu-sol-therm-021-case_1.t9a	1.0000±0.0032	-	1.0043±0.0003	1.00229±0.00045	-
				pu-sol-therm-021-CASE_3.T9A	1.0000±0.0065	-	1.0044±0.0004	1.00337±0.00047	1.00334±0.00044
		Cylinder	Water	pu-sol-therm-018-case_9	1.0000±0.0034	-	1.0031±0.0005	1.00207±0.00032	-
				pu-sol-therm-034-case_01	1.0000±0.0062	-	0.9999±0.0004	0.99776±0.00040	-

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

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Additional Benchmarks

		Case	Benchmark	ENDF/B-VII R. D. Mosteller[*]	NEA JEFF3.1[**]	NEA JEFF3.1.1[**]	This work NEA JEFF3.1.2
PU	**Thermal**	PU-SOL-THERM-009 (48-inch sphere of plutonium nitrate solution)	1.00030 (330)	1.01910 (20)	1.01515 (49)	1.01003 (49)	1.01107 (48)
			• Same sphere as for ORNL-10 (HEU) and ORNL-11 (U233) Benchmarks • Very thermal spectra with vey little leakage • **Cross sections for Pu239 should be re-examined in the deep thermal range**				
HEU	**Fast**	HEU-MET-FAST-73 (Unmoderated ZEUS benchmark)	1.00120 (150)	1.00800 (30)	1.00849 (26)	1.00759 (29)	1.00763(28)
			• Benchmark contains no moderator and therefore has a fast spectrum • **Fast cross sections for Cu should be reviewed**				
HEU	**Thermal**	HEU-SOL-THERM-004_case1 (Heavy water solutions, reflected spheres)	1.00000 (330)	0.98390 (40)	0.98438 (38)	0.98559 (39)	0.98482(47)
			• **Improvement for cases with deuterium**				
SPEC	**Thermal**	SPEC-MET-FAST-08 (Neptunium sphere reflected by HEU)	1.00190 (360)	0.99240 (30)	0.99177 (24)	0.98940 (23)	0.99007(25)
			• **Fast cross sections for Np-237 should be reviewed**				

In summary ...

1) JEFF-3.1.2 processed with NJOY99.364 in ACE format for the general purpose and thermal scattering libraries.

- ACE files with graphs and documentation from the Quality Assurance procedure
- ACE libraries at 300K, …, 1800K for the General Purpose File and additional temperatures for Thermal Scattering data

2) JEFF-3.1.2, ENDF/B-VII.1and TENDL-2011 processed into:

- PENDF format to be used in JANIS
- BOXER format to be used in JANIS

3) Updated Covariance evaluated files for U233 and Nb93

4) Additional patches for NJOY and problems processing TENDL2011 are reported